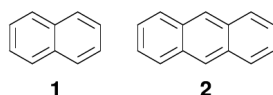


# Benchmarking the SPARC software program for estimating solubilities of naphthalene and anthracene in organic solvents

Sierra Rayne<sup>a,\*</sup> and Kaya Forest<sup>b</sup>

The solubility of polyaromatic hydrocarbons (PAHs) and their derivatives in organic solvents is of substantial interest for the upstream and downstream petroleum sectors [1-4]. Knowledge of this physico-chemical property helps guide the development and optimization of existing and proposed extraction and processing operations. In addition to extensive experimental work determining the solubilities of various PAHs (see, e.g., ref. [5-21]), a number of studies have developed quantitative structure-property relationships (QSPRs) and employed associated software programs (see, e.g., ref. [22-28]) for predicting the solubility of these compounds in a wide range of solvent systems.

To date, despite its broad applications towards predicting the partitioning behavior and reactivity of various organic compounds, the SPARC software program [29-36] has not been previously benchmarked for its capacity to estimate the solubility of representative PAHs in organic solvents. Consequently, in the current work we investigate the ability of SPARC to predict the solubilities of naphthalene (1) and anthracene (2) (Figure 1) in a range of organic solvents at various temperatures.



**Fig. 1.** Structures of naphthalene (1) and anthracene (2).

Mole fraction solubilities ( $\log_{10} X_A^{\text{sat}}$ ) of 1 and 2 were estimated using SPARC (August 2011 release w4.6.1646-s4.6.1646; <http://ibmic2.chem.uga.edu/sparc/>) with the default settings and solvent profiles. We have previously examined the ability of this program to estimate the  $\text{pK}_a$  values, hydrolysis rate constants, and partitioning behavior of several classes of organic compounds [37-46].

We began our studies using the  $X_A^{\text{sat}}$  of naphthalene obtained in chloroform, t-butanol, cyclohexanol, 2-propanol, 1-propanol, and ethanol at 40°C under atmospheric pressure (Table 1). Poor agreement between the experimental and SPARC predicted  $X_A^{\text{sat}}$  was found for t-butanol, cyclohexanol, and 2-propanol (errors of +0.78, +0.41, and +0.45  $\log_{10}$  units, respectively), with reasonable  $X_A^{\text{sat}}$  agreement for chloroform, 1-propanol, and ethanol (errors of +0.11, -0.15, and -0.02  $\log_{10}$  units, respectively).

**Table 1.** Comparison between experimental and SPARC estimated mole fraction solubilities ( $\log_{10} X_A^{\text{sat}}$ ) of naphthalene in selected organic solvents at 40°C under atmospheric pressure.

	expt.	SPARC
chloroform	-0.33 [47]	-0.22
t-butanol	-1.00 [47]	-0.22
cyclohexanol	-0.63 [47]	-0.22
2-propanol	-1.12 [47]	-0.67
1-propanol	-1.03 [47]	-1.28
ethanol	-1.14 [47]	-1.16

However, a recurring problem with SPARC appears to be its inconsistency in reproducing results between different sessions of the online program. For example, during one session,  $X_A^{\text{sat}}$  of -0.16,

-0.16, -0.16, -0.16, -0.94, and -0.84 were obtained for chloroform, t-butanol, cyclohexanol, 2-propanol, 1-propanol, and ethanol at 40°C, respectively. Later the same day, different corresponding  $X_A^{\text{sat}}$  values of -0.22, -0.22, -0.22, -0.67, -1.28, and -1.16 were obtained. We have previously reported on the temporal instability of the SPARC program for predicting partitioning properties [40]. Several concerns arise from this software behavior. The first issue is that solvents with such widely differing physico-chemical properties as chloroform, t-butanol, and cyclohexanol should not have equivalent predicted  $X_A^{\text{sat}}$  to two significant figures for PAHs. Additionally, temporal inconsistencies in the prediction performance of any software program renders it of little utility, and suggests substantial code errors as the source of the anomalous and unpredictable responses.

We then considered the solubility behavior of naphthalene in a suite of additional organic solvents of varying polarity and for which broad temperature range specific  $X_A^{\text{sat}}$  values were available (Table 2). With the single exception of methanol, SPARC overestimates the solubility of naphthalene in all solvents (i.e.,  $\log_{10} X_{A,\text{SPARC}}^{\text{sat}} > \log_{10} X_{A,\text{expt}}^{\text{sat}}$ ). Similarly, with the exception of methanol, the SPARC prediction performance improves with increasing temperature, as the solute becomes more soluble in the solvent. While the errors in predicted versus experimental  $\log_{10} X_A^{\text{sat}}$  are typically on the order of several tenths of a  $\log_{10}$  unit at low temperatures, at higher temperatures the error is reduced (with the exception of methanol) to <0.1  $\log_{10}$  units.

**Table 2.** Comparison between experimental and SPARC estimated mole fraction solubilities ( $\log_{10} X_A^{\text{sat}}$ ) of naphthalene in selected organic solvents at various temperatures under atmospheric pressure.

benzene			chlorobenzene		
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
6.1	-0.76 [48]	-0.31	4.2	-0.73 [48]	-0.32
15.0	-0.65 [48]	-0.27	8.8	-0.68 [48]	-0.30
21.7	-0.57 [48]	-0.24	22.1	-0.53 [48]	-0.24
29.1	-0.49 [48]	-0.20	29.4	-0.46 [48]	-0.20
39.6	-0.38 [48]	-0.16	40.0	-0.35 [47]	-0.16
40.0	-0.37 [47]	-0.16	42.8	-0.33 [48]	-0.14
48.8	-0.28 [48]	-0.12	49.0	-0.27 [48]	-0.12
61.2	-0.16 [48]	-0.071	62.6	-0.15 [48]	-0.066
methanol			acetone		
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
0.8	-1.97 [48]	-2.33	6.3	-0.90 [48]	-0.69
13.5	-1.79 [48]	-2.08	14.3	-0.78 [48]	-0.28
26.3	-1.59 [48]	-1.85	24.2	-0.64 [48]	-0.23
33.6	-1.48 [48]	-1.72	32.6	-0.52 [48]	-0.19
40.0	-1.36 [47]	-1.61	39.3	-0.44 [48]	-0.16
43.9	-1.29 [48]	-1.55	40.0	-0.42 [47]	-0.16
56.7	-0.99 [48]	-1.34	47.2	-0.33 [48]	-0.13
68.4	-0.41 [48]	-1.14	58.5	-0.21 [48]	-0.081
74.3	-0.086 [48]	-1.03	69.5	-0.094 [48]	-0.039
n-butanol			nitrobenzene		
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
11.7	-1.31 [48]	-1.23	2.9	-0.79 [48]	-0.59
22.0	-1.24 [48]	-1.04	13.8	-0.66 [48]	-0.28
31.6	-1.09 [48]	-0.80	24.0	-0.54 [48]	-0.23
40.0	-0.94 [47]	-0.16	40.0	-0.36 [47]	-0.16
46.5	-0.80 [48]	-0.13	45.3	-0.31 [48]	-0.14
56.9	-0.56 [48]	-0.088	60.2	-0.17 [48]	-0.075
68.1	-0.22 [48]	-0.045	65.3	-0.12 [48]	-0.055
76.0	-0.04 [48]	-0.015	71.8	-0.070 [48]	-0.031

**Table 2 cont'd.**

aniline			n-hexane		
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
0.6	-1.16 [48]	-0.34	8.7	-1.21 [48]	-0.45
10.6	-0.99 [48]	-0.29	14.8	-1.10 [48]	-0.41
22.0	-0.81 [48]	-0.24	19.5	-1.02 [48]	-0.38
29.9	-0.68 [48]	-0.20	27.7	-0.88 [48]	-0.33
37.4	-0.56 [48]	-0.17	36.1	-0.73 [48]	-0.28
40.0	-0.51 [47]	-0.16	40.0	-0.65 [47]	-0.25
50.8	-0.35 [48]	-0.11	45.8	-0.54 [48]	-0.13
60.8	-0.20 [48]	-0.072	57.9	-0.30 [48]	-0.084
65.4	-0.15 [48]	-0.055	64.6	-0.18 [48]	-0.058
74.4	-0.055 [48]	-0.021	72.5	-0.072 [48]	-0.028
carbon tetrachloride			toluene		
T (°C)	expt.	SPARC	T (°C)	expt.	SPARC
0.4	-0.92 [48]	-0.36	8.2	-0.74 [48]	-0.31
6.0	-0.84 [48]	-0.32	17.3	-0.63 [48]	-0.26
13.0	-0.75 [48]	-0.28	34.8	-0.43 [48]	-0.18
19.5	-0.66 [48]	-0.25	40.0	-0.37 [47]	-0.16
28.2	-0.55 [48]	-0.21	43.9	-0.33 [48]	-0.14
39.5	-0.41 [48]	-0.16	52.1	-0.25 [48]	-0.11
40.0	-0.40 [47]	-0.16	67.4	-0.13 [48]	-0.047
46.9	-0.32 [48]	-0.13			
58.3	-0.20 [48]	-0.082			
64.8	-0.14 [48]	-0.057			
72.4	-0.067 [48]	-0.028			

Although the SPARC prediction errors for the solubilities of naphthalene at low temperatures in these organic solvents are larger than desired, they were sufficiently modest to warrant an examination into the solubilities of the next highest member of the [n]acene PAH series – anthracene – in various organic solvents (Tables 3 and 4). For this larger PAH, we find generally poor SPARC prediction performance at both low and moderately elevated temperatures, with  $\log_{10} X_A^{\text{sat}}$  errors (always positive with the exceptions of ethylene glycol and 2,2,2-trifluoroethanol) typically on the order of one  $\log_{10}$  unit or higher. In each of the solvents for which multiple temperature comparisons were made (toluene, 2-propanol, and n-heptane), the prediction errors all decline with increasing temperature, but not to the extent required to obtain reliable  $\log_{10} X_A^{\text{sat}}$  estimates.

**Table 3.** Comparison between experimental and SPARC estimated mole fraction solubilities ( $\log_{10} X_A^{\text{sat}}$ ) of anthracene in selected organic solvents at 25°C under atmospheric pressure.

solvent	expt.	SPARC
n-nonane	-2.68 [49]	-1.02
n-decane	-2.63 [49]	-1.02
chloroform	-1.96 [49]	-1.31
dichloromethane	-2.03 [49]	-1.17
chlorobenzene	-2.00 [49]	-0.80
methanol	-3.61 [49]	-3.21
ethanol	-3.34 [49]	-2.37
1-hexanol	-2.83 [49]	-1.70
cyclopentanol	-2.88 [49]	-2.07
ethylene glycol	-4.15 [49]	-4.86
2,2,2-trifluoroethanol	-4.06 [49]	-5.27
acetonitrile	-3.08 [49]	-2.26
benzonitrile	-2.07 [49]	-0.82
N,N-dimethylformamide	-2.11 [49]	-1.40
N,N-dimethylacetamide	-1.90 [49]	-1.16

**Table 4.** Comparison between experimental and SPARC estimated mole fraction solubilities ( $\log_{10} X_A^{\text{sat}}$ ) of anthracene in selected organic solvents at various temperatures under atmospheric pressure.

solvent	Temperature (°C)	expt.	SPARC
		$\log_{10} X_A^{\text{sat}}$	$\log_{10} X_A^{\text{sat}}$
toluene	20.0	-2.21 [50]	-1.07
	25.0	-2.14 [50]	-1.05
	30.0	-2.07 [50]	-1.00
	35.0	-1.98 [50]	-0.96
	40.0	-1.95 [50]	-0.93
	45.0	-1.85 [50]	-0.89
2-propanol	50.0	-1.80 [50]	-0.85
	20.0	-3.72 [50]	-1.90
	25.0	-3.43 [50], -3.39 [51], -3.47 [52]	-1.85
	30.0	-3.37 [50], -3.36 [52]	-1.75
	35.0	-3.24 [50], -3.21 [52]	-1.68
	40.0	-3.13 [50], -3.09 [52]	-1.61
n-heptane	45.0	-3.13 <sup>a</sup> [50]	-1.53
	50.0	-2.96 [50]	-1.47
	20.0	-2.92 [50]	-1.09
	25.0	-2.87 [50], -2.80 [53]	-1.05
	30.0	-2.73 [50]	-1.00
	35.0	-2.75 [50]	-0.96
	40.0	-2.63 [50]	-0.92
	45.0	-2.49 [50]	-0.88
	50.0	-2.46 [50]	-0.84

<sup>a</sup> reported experimental  $X_A^{\text{sat}}$  value in ref. [50] is suspect as these authors report no change in  $X_A^{\text{sat}}$  between 40°C and 45°C, in contrast to expectations and the general trend between 20°C and 50°C.

Overall, the results suggest that the SPARC software program is currently not suitable for accurately predicting the solubilities of representative PAHs relevant for the petroleum sector in various organic solvents.

## References and Notes

- <sup>a</sup> Chemologica Research, PO Box 74, 318 Rose Street, Mortlach, Saskatchewan, Canada, S0H 3E0  
<sup>b</sup> Department of Environmental Engineering, Saskatchewan Institute of Applied Science and Technology, Palliser Campus, PO Box 1420, 600 6th Avenue NW, Moose Jaw, Saskatchewan, Canada, S6H 4R4

\* Corresponding author: rayne.sierra@gmail.com

- [1] Fahim MA, Al-Sahhaf TA & Elkilani A. *Fundamentals of petroleum refining*. Elsevier, New York, 2010.  
[2] Wauquier JP & Favennec JP. *Petroleum refining: Refinery operation and management*. Editions TECHNIP, Paris, 2001.  
[3] Gary JH & Handwerk GE. *Petroleum refining: Technology and economics*. CRC Press, Boca Raton, FL, 2001.  
[4] Le Page JF, Chatila SG & Davidson M. *Resid and heavy oil processing*. Editions TECHNIP, Paris, 1992.  
[5] Judy CL, Pontikos NM & Acree WE. Solubility of pyrene in binary solvent mixtures containing cyclohexane. *J. Chem. Eng. Data* (1987) **32**: pp. 60-62.  
[6] Hernandez CE, Coym KS, Roy LE, Powell JR & Acree WE. Solubility of pyrene in binary (alkane + 2-butanol) solvent mixtures. *J. Chem. Thermodyn.* (1998) **30**: pp. 37-42.  
[7] Zvaigzne AI & Acree WE. Solubility of pyrene in binary alkane + 1-propanol and alkane + 2-propanol solvent mixtures. *J. Chem. Eng. Data* (1993) **38**: pp. 393-395.  
[8] Wallach JR, Tucker SA, Oswalt BM, Murrall DJ & Acree WE.

Solubility of pyrene in binary solvent mixtures containing dibutyl ether. *J. Chem. Eng. Data* (1989) **34**: pp. 70-73.

[9] McHale MER, Coym KS, Fletcher KA & Acree WE. Solubility of pyrene in binary alcohol + 2-methyl-2-butanol solvent mixtures at 299.2 K. *J. Chem. Eng. Data* (1997) **42**: pp. 511-513.

[10] Debase EM & Acree WE. Solubility of pyrene in ternary propanol + butanol + cyclohexane solvent mixtures at 299.15 K. *J. Chem. Eng. Data* (2001) **46**: pp. 991-993.

[11] Zvaigzne AI, McHale MER, Powell JR, Kauppila ASM & Acree WE. Solubility of anthracene and pyrene in binary alcohol + alcohol solvent mixtures. *J. Chem. Eng. Data* (1995) **40**: pp. 1273-1275.

[12] Zvaigzne AI & Acree WE. Solubility of anthracene in binary alkane + 3-methyl-1-butanol solvent mixtures. *J. Chem. Eng. Data* (1994) **39**: pp. 708-710.

[13] Marthandan MV & Acree WE. Solubility of anthracene in binary solvent mixtures containing dibutyl ether. *J. Chem. Eng. Data* (1987) **32**: pp. 301-303.

[14] Zvaigzne AI, Wolfe J & Acree WE. Solubility of anthracene in binary alkane + 2-methyl-1-propanol solvent mixtures. *J. Chem. Eng. Data* (1994) **39**: pp. 541-543.

[15] Jouyban A, Khoubnasabjafari M, Chan HK, Clark BJ & Acree WE. Solubility prediction of anthracene in mixed solvents using a minimum number of experimental data. *Chem. Pharm. Bull.* (2002) **50**: pp. 21-25.

[16] Ali SH. Measurement and prediction of pyrene solubility in pure, binary, ternary and quaternary solvent systems. *Fluid Phase Equilib.* (2008) **264**: pp. 29-44.

[17] Ali SH & Al-Rashed OA. Solubility of pyrene in simple and mixed solvent systems. *Fluid Phase Equilib.* (2009) **281**: pp. 133-143.

[18] Pribyla KJ, Spurgin MA, Chuca I & Acree WE. Solubility of anthracene in ternary 1,4-dioxane + alcohol + cyclohexane solvent mixtures at 298.15 K. *J. Chem. Eng. Data* (2000) **45**: pp. 971-973.

[19] Pribyla KJ & Acree WE. Solubility of anthracene in ternary dibutyl ether + alcohol + heptane solvent mixtures at 298.15 K. *J. Chem. Eng. Data* (1999) **44**: pp. 1259-1261.

[20] Powell JR, Miller BJ & Acree WE. Solubility of anthracene in binary alcohol + 1,4-dioxane solvent mixtures. *J. Chem. Eng. Data* (1995) **40**: pp. 1124-1126.

[21] Powell JR & Acree WE. Solubility of anthracene in binary alcohol + dibutyl ether solvent mixtures. *J. Chem. Eng. Data* (1995) **40**: pp. 914-916.

[22] Acree WE & Rytting JH. Solubility in binary solvent systems. IV. Prediction of naphthalene solubilities using the UNIFAC group contribution model. *Int. J. Pharm.* (1983) **13**: pp. 197-204.

[23] Acree WE & Abraham MH. Solubility predictions for crystalline polycyclic aromatic hydrocarbons (PAHs) dissolved in organic solvents based upon the Abraham general solvation model. *Fluid Phase Equilib.* (2002) **201**: pp. 245-258.

[24] Acree WE, Zvaigzne AI & Tucker SA. Thermochemical investigations of hydrogen-bonded solutions: Development of a predictive equation for the solubility of anthracene in binary hydrocarbon. *Fluid Phase Equilib.* (1994) **92**: pp. 233-253.

[25] Powell JR, McHale MER, Kauppila ASM, Acree WE, Flanders PH, Varanasi VG & Campbell SW. Prediction of anthracene solubility in alcohol + alkane solvent mixtures using binary alcohol + alkane VLE data. Comparison of Kretschmer-Wiebe and mobile order models. *Fluid Phase Equilib.* (1997) **134**: pp. 185-200.

[26] Ali SH, Al-Mutairi FS & Fahim MA. Solubility of polycyclic aromatics in binary solvent mixtures using activity coefficient models. *Fluid Phase Equilib.* (2005) **230**: pp. 176-183.

[27] Acree WE & Abraham MH. Solubility predictions for crystalline nonelectrolyte solutes dissolved in organic solvents based upon the Abraham general solvation model. *Can. J. Chem.* (2001) **79**: pp. 1466-1476.

[28] Hansen HK, Riverol C & Acree WE. Solubilities of anthracene, fluoranthene and pyrene in organic solvents: Comparison of

calculated values using UNIFAC and modified UNIFAC (Dortmund) models with experimental data and values using the mobile order theory. *Can. J. Chem. Eng.* (2000) **78**: pp. 1168-1174.

[29] Carreira LA, Hilal S & Karickhoff SW. "Estimation of chemical reactivity parameters and physical properties of organic molecules using SPARC." In *Theoretical and computational chemistry: quantitative treatment of solute/solvent interactions*. Politzer P & Murray JS (Eds.), Elsevier, New York, 1994, pp. 291-353.

[30] Hilal SH, Bornander LL & Carreira LA. Hydration equilibrium constants of aldehydes, ketones and quinazolines. *QSAR Comb. Sci.* (2005) **24**: pp. 631-638.

[31] Hilal SH, Carreira LA & Karickhoff SW. Prediction of the solubility, activity coefficient, gas/liquid and liquid/liquid distribution coefficients of organic compounds. *QSAR Comb. Sci.* (2004) **23**: pp. 709-720.

[32] Hilal SH, Karickhoff SW & Carreira LA. A rigorous test for SPARC's chemical reactivity models: Estimation of more than 4300 ionization pK<sub>a</sub>s. *Quant. Struct.-Act. Relat.* (1995) **14**: pp. 348-355.

[33] Hilal SH, Karickhoff SW & Carreira LA. Prediction of the vapor pressure boiling point, heat of vaporization and diffusion coefficient of organic compounds. *QSAR Comb. Sci.* (2003) **22**: pp. 565-574.

[34] Hilal SH, Karickhoff SW, Carreira LA & Shrestha BP. Estimation of carboxylic ester hydrolysis rate constants. *QSAR Comb. Sci.* (2003) **22**: pp. 917-925.

[35] Hilal SH, Saravananaraj AN, Whiteside T & Carreira LA. Calculating physical properties of organic compounds for environmental modeling from molecular structure. *J. Comput. Aided Mol. Des.* (2007) **21**: pp. 693-708.

[36] Hilal SH. *Estimation of hydrolysis rate constants of carboxylic acid ester and phosphate ester compounds in aqueous systems from molecular structure by SPARC*. Ecosystems Research Division, National Exposure Research Laboratory, United States Environmental Protection Agency, Athens, GA, USA, 2006.

[37] Rayne S & Forest K. A new class of perfluorinated acid contaminants: Primary and secondary substituted perfluoroalkyl sulfonamides are acidic at environmentally and toxicologically relevant pH values. *J. Environ. Sci. Health A* (2009) **44**: pp. 1388-1399.

[38] Rayne S & Forest K. Perfluoroalkyl sulfonic and carboxylic acids: A critical review of physicochemical properties, levels and patterns in waters and waste waters, and treatment methods. *J. Environ. Sci. Health A* (2009) **44**: pp. 1145-1199.

[39] Rayne S & Forest K. An assessment of organic solvent based equilibrium partitioning methods for predicting the bioconcentration behavior of perfluorinated sulfonic acids, carboxylic acids, and sulfonamides. *Nature Precedings* (2009) <http://hdl.handle.net/10101/npre.2009.3256.2>.

[40] Rayne S & Forest K. D<sub>ow</sub> and K<sub>aw,eff</sub> vs. K<sub>ow</sub> and K<sub>aw</sub> degrees: Acid/base ionization effects on partitioning properties and screening commercial chemicals for long-range transport and bioaccumulation potential. *J. Environ. Sci. Health A* (2010) **45**: pp. 1550-1594.

[41] Rayne S & Forest K. A comparative assessment of octanol-water partitioning and distribution constant estimation methods for perfluoroalkyl carboxylates and sulfonates. *Nature Precedings* (2009) <http://hdl.handle.net/10101/npre.2009.3282.2>.

[42] Rayne S & Forest K. ADME/Tox WEB in silico predictions of longer chain perfluoroalkyl carboxylic acid pK<sub>a</sub> values are more accurate than other computational methods. *Nature Precedings* (2009) <http://hdl.handle.net/10101/npre.2009.2936.1>.

[43] Rayne S & Forest K. Congener specific organic carbon normalized soil and sediment-water partitioning coefficients for the C<sub>1</sub> through C<sub>8</sub> perfluorinated alkylsulfonic and alkylcarboxylic acids. *J. Environ. Sci. Health A* (2009) **44**: pp. 1374-1387.

[44] Rayne S & Forest K. Re-evaluating the list of high-production chemicals predicted to become Arctic contaminants. *Nature Precedings* (2010) doi:10.1038/npre.2010.4436.1.

- [45] Rayne S & Forest K. Modeling the hydrolysis of perfluorinated compounds containing carboxylic and phosphoric acid ester functions and sulfonamide groups. *J. Env. Sci. Health A* (2010) **45**: pp. 432-446.
- [46] Rayne S, Forest K & Friesen KJ. Estimated congener specific gas phase atmospheric behavior and fractionation of perfluoroalkyl compounds: Rates of reaction with atmospheric oxidants, air-water partitioning, and wet/dry deposition lifetimes. *J. Environ. Sci. Health A* (2009) **44**: pp. 936-954.
- [47] Martin A, Wu PL, Adjei A, Beerbower A & Prausnitz JM. Extended Hansen solubility approach: Naphthalene in individual solvents. *J. Pharmaceut. Sci.* (1981) **70**: pp. 1260-1264.
- [48] Ward HL. The solubility relations of naphthalene. *J. Phys. Chem.* (1926) **30**: pp. 1316-1333.
- [49] Roy LE, Hernandez CE & Acree WE. Solubility of anthracene in organic nonelectrolyte solvents. Comparison of observed versus predicted values based upon mobile order theory. *Polycycl. Aromat. Comp.* (1999) **13**: pp. 105-116.
- [50] Al-Sharrah GK, Ali SH & Fahim MA. Solubility of anthracene in two binary solvents containing toluene. *Fluid Phase Equilib.* (2002) **193**: pp. 191-201.
- [51] Powell JR, Coym KS & Acree WE. Solubility of anthracene in binary alcohol + 2-methoxyethyl ether solvent mixtures. *J. Chem. Eng. Data* (1997) **42**: pp. 395-397.
- [52] Cepeda EA & Diaz M. Solubility of anthracene and anthraquinone in acetonitrile, methyl ethyl ketone, isopropol alcohol and their mixtures. *Fluid Phase Equilib.* (1996) **121**: pp. 267-272.
- [53] Roy LE, Hernandez CE, Reddy GD, Sanders JT, Deng T, Tuggle MB & Acree WE. Solubility of anthracene in binary alkane + 2-ethyl-1-hexanol and alkane + 1-pentanol solvent mixtures at 298.2 K. *J. Chem. Eng. Data* (1998) **43**: pp. 493-495.